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General Software Corp., Landover, MD

Prepared for

Environmental Protection Agency, Washington, DC

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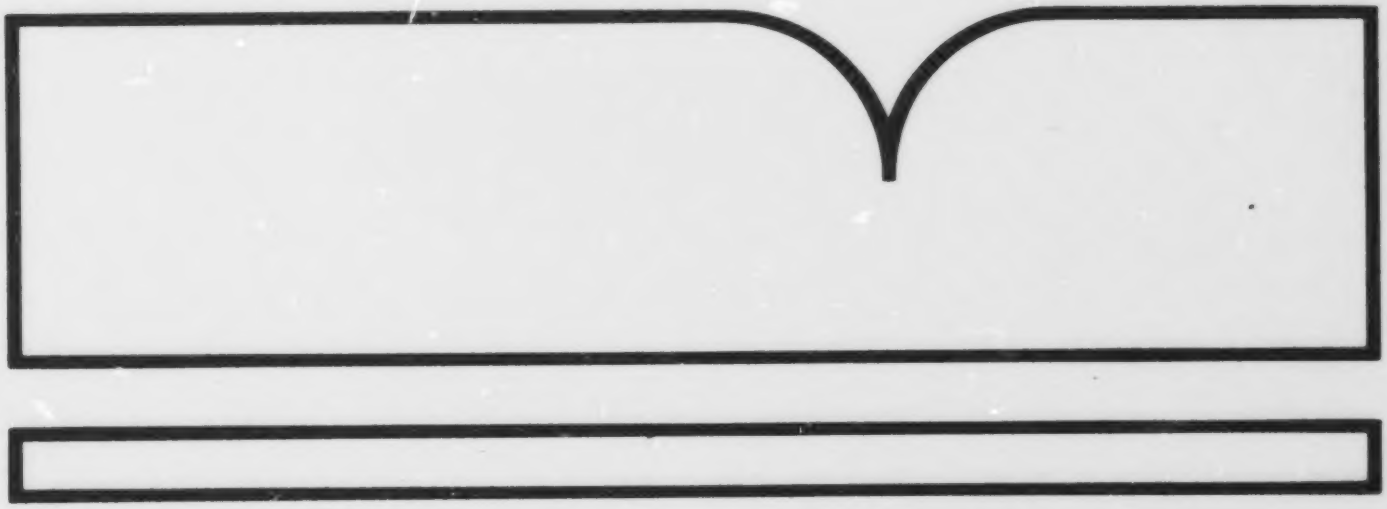

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USER'S GUIDE TO AT123D EXECUTION USING THE DATA MANAGEMENT SUPPORTING SYSTEMS AT123DIN AND AT123DOUT

Prepared for:

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF PESTICIDES AND TOXIC SUBSTANCES
EXPOSURE EVALUATION DIVISION
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Detailed procedures required to execute AT123D through the use of two data management systems. Intended to be a comprehensive guide for users who have no specialized computer knowledge.

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I. INTRODUCTION

AT123D is a generalized analytical transient one-, two-, and/or three-dimensional computer model designed for estimating the rate of pollutant (radioactive, chemical, or thermal) transport/transformation in a groundwater system (i.e., the saturated zone). It was originally developed by G.T. Yeh (1981) of the Oak Ridge National Laboratory to provide "the engineering community with a ready tool for the preliminary assessment of waste disposal sites". In the search for closed-form solutions to the partial differential equations describing the groundwater flow and transport phenomena, the application of the Green's function is used to its optimum advantage. As a result, the model has many optional capabilities and accepts a variety of source release patterns and configurations.

Under the auspices of the modeling team in the Office of Pesticides and Toxic Substances (OPTS) of the Environmental Protection Agency (EPA). the General Software Corporation (GSC) has implemented two data management systems, one for the input and one for the output, in support of the AT123D modeling operation. The input data management system (AT123DIN) uses interactive prompts to assist you, the user, in the preparation of the model input file. Through AT123DIN, you may use various commands to perform efficient data entry, manipulation, and editing. The output data management system (AT123DOUT) provides you with the option of storing the AT123D output parameters in the Graphical Exposure Modeling System (GEMS) (GSC 1982) so that these parameters can be further analyzed, using available graphical, statistical, and tabular display facilities.

The purpose of this document is to describe in detail the procedures required to execute AT123D through the use of the two data management systems. It is intended as a comprehensive guide for users who have no specialized computer knowledge. However, a working knowledge of GEMS, through which AT123D is executed, is necessary for making more efficient use of the AT123D model. Only a brief description of AT123D's input data file requirements is presented to facilitate the subsequent discussions. More detailed model information is contained in the original AT123D manual (Yeh, 1981).

II. AT123D DATA REQUIREMENT

There are a total of nine (9) input data groups required by AT123D. The 9th group is optional, depending on the time dependency of the pollutant source release rate you specify. These groups are defined and presented in Appendix 3.

In the preparation of these AT123D input data groups, the following considerations must be noted.

1. The maximum values of NX, NY, and NZ allowed by the current AT123D version are 15, 10, and 10, respectively.

2.. The allowable maximum number of time points where the solutions are calculated is 20. Since the model solutions at time=0.0 hour are always given, you need to ensure that the results of

((NEDTI - NBGTI)/NPRINT +1)

are less than or equal to 19.

3. The number of eigenvalues required for numerical series evaluations (NROOT) varies depending on your input data characteristics. A warning message, such as "WARNING: SERIESY AT Y=20 TIMED=35280 NEEDS MORE TERMS", will appear in the output if the assigned NROOT value is too small. A suggested approach is to start with NROOT=400. Raise the value of NROOT if the warning message appears.

4. The value of IBUG should always be set to "0" for your production runs. As such, AT123DIN will automatically set IBUG=0 and you will not be able to access this value through the use of AT123DIN.

III. GUIDE TO AT123D EXECUTION AND DATA MANAGEMENT

A. Access to AT123D

You can access AT123D through the Graphical Exposure Modeling System (GEMS). The GEMS host computer is a Digital Equipment Corporation VAX 11/780, located at EPA's National Computer Center (NCC) in Research Triangle Park, North Carolina.

It is assumed that you are familiar with the log-on procedures of the VAX system and are able to invoke GEMS (Consult User's Guide to GEMS, if not). After you have made connection, the two steps required to gain access to AT123D in GEMS are:

ENTER AN OPERATION: M <CR>*

ENTER MODEL NAME: AT123D <CR>

* Where M stands for MODELING and <CR> stands for pressing the carriage return key on the terminal.

B. Major Control Options in AT123D Execution

When you make an AT123D run using AT123DIN and AT123DOUT, you have the following options:

1. Source of input data used by AT123DIN

   (a) You can create a new input data file by editing an AT132DIN-supplied dataset having default values for all input variables.

(b) You can create a new input data file by editing the values contained in an existing input data file.

(c) You can call in an existing input data file (instead of creating a new one) for immediate AT123D execution.

For (a), a list of default values used in the AT123DIN input default data file is given in Appendix 3.

For (b) and (c), you need to know the file name of your existing input data file.

Note: In general, the AT123D default dataset is based on a 5-year continuous pollutant loading scenario from a 1 meter square area source located at the groundwater surface. The aquifer has infinite width and depth. All soil-dependent parameters are based on typical values for silty soil. The space coordinates for solution are chosen as 0 to 50 meters at 10-meter intervals in the x direction, 0 to 10 meters longitudinally from both sides of the source at 5-meter intervals in the Y direction, and 0 to 20 meters at 5-meter intervals in the Z direction (depth). The time intervals between computed solutions are 1 year for a duration of 5 years.

2. Type of dataset stored in GEMS by AT123DOUT

There are three types of datasets you can store in GEMS for later graphical, statistical, or tabular analysis:

(i) Dataset containing the predicted pollutant concentrations vs. the time values (you can use it to plot a scatter diagram showing the variation of pollutant concentration in time). Since AT123D is a three-dimensional, time-dependent model, AT123DOUT will prompt you to specify the values of x-coordinate, y-coordinate, and z-coordinate.

(ii) Dataset containing the predicted pollutant concentrations vs. the values of x-coordinate (you can use it to plot a scatter diagram showing the variation of pollutant concentration along the x-direction). Since AT123D is a three-dimensional, time-dependent model, AT123DOUT will prompt you to specify the values of time, y-coordinate, and z-coordinate.

(iii) Dataset containing all the output parameters generated by AT123D. This is a relatively large dataset, which you can use to obtain desired smaller datasets (including those described in (i) and (ii)) through the use of GEMS EXTRACT and FILTER functions.

You can request more than one dataset for type (i) or type (ii) at different locations and/or time values. However, the total combined number of datasets for types (i), (ii), and (iii) together should not be greater than 10 for each AT123D run.

As presented above, it is clear that you need to consider the following questions at the outset and throughout the process of AT123D execution:

- o Which of the following will I use to get my input data file?
  - by creating one through editing a default file?
  - by creating one through editing an existing file?
  - by directly calling in an existing file for execution?
- o If I use AT123DOUT support, what type of dataset do I want to store in GEMS? and how many?

A flowchart outlining the relative sequence of the above control options is presented in Figure 1. As shown, the entire process can be divided into four optional blocks which will be discussed below.

C. Structured AT123D Execution Using AT123DIN and AT123DOUT

To facilitate the following discussion, this section will be presented in terms of the four optional blocks as shown in Figure 1.

(1) Block 1

The flow of execution enters this block if you have elected to create the input data file (node 1). The input data file can be created either by editing an existing file (node 3) or by editing the default data file (node 4). Node 5, the main portion of AT123DIN, guides you interactively through efficient data entry, manipulation, and editing procedures. You are provided with the following AT123DIN commands:

ALL	BACK	BRIEF	CANCEL	CLEAR	<CR>	DONE
EXIT	HELP	MENU	NOBRIEF	REVIEW		

A detailed list of command descriptions is presented in Table 1.

Throughout the entire Block 1 process, you are guided by self-explanatory prompts provided by AT123DIN. You can respond with brief answers or use the above listed commands to control the progress of the process. The use of AT123DIN and its commands can be illustrated best by Appendix 1, which contains a step-by-step example side-marked with

demonstration comments. You are advised to follow this example carefully in order to make efficient use of AT123DIN.

(2) Block 2

This block represents the original AT123D data file input fashion in that it prompts you to input the run-ready data file required for direct AT123D execution. The flow of execution will enter this branch if you choose not to create a new data file (node 1) through the use of AT123DIN. An example is given in Appendix 2 to illustrate the use of this block.

(3) Block 3

This block represents the use of the GSC-developed AT123D output data management system, AT123DOUT, which allows you to store a number of AT123D output datasets (in terms of the three different types as specified previously) in GEMS so that later you can use GEMS' capabilities for output graphical display, statistical analysis, and tabular presentation. The variables contained in a dataset vary depending on the type of dataset you have requested. A listing of the variables included in each dataset type is presented below.

Type (i): VAR ID, VAR NAME, VAR UNIT, TIME, POLLUT, XPOINT, YPOINT, ZPOINT

Type (ii): VAR ID, VAR NAME, VAR UNIT, XDIST, POLLUT, TPOINT, YPOINT, ZPOINT

Type (iii): VAR ID, VAR NAME, VAR UNIT, ISOIFO1, ISOIFO2, TIME, XDIM, YDIM, ZDIM, POLLUT, TITLE, NX, NY, NZ, NROOT, NBGTI, NEDTI, NPRINT, INSTAN, NSOUS, INTER, ICASE, DEPTH, WIDTH, RL1, RL2, RB1, RB2, RH1, RH2, POR, HCOND, HGRAD, AELONG, ATRANV, AVERT1, AKD, AKE, AMTAU, RAMADA, RHOB, RHOW, ACCU, DT, TDISP, Q, RETARD, UF, AKX, AKY, AKZ

Where

VAR ID: Variable identification code (used to call out the variable needed).

VAR NAME: Descriptive variable definition.

VAR UNIT: Variable unit definition.

TIME: Time values estimated using NBGTI, NEDTI, and DT.

POLLUT: Estimated pollutant magnitudes.

XPOINT: Value of the x-coordinate you specify when requesting the Type (i) dataset.

YPOINT: Value of the y-coordinate you specify when requesting the Type (i) or Type (ii) dataset.

ZPOINT: Value of the z-coordinate you specify when requesting the Type (i) or Type (ii) dataset.

XDIST: Value of x-coordinates where solutions are estimated (identical to XDIM).

TPOINT: The time value specified by you in requesting the Type (ii) dataset.

ISOIF01 & ISOIF02: Information needed by GEMS' isopleth mapping routine. You have no need of these variables.

OTHERS: The definitions for the other variables are given in Appendix 3 of this document and also in the original AT123D manual (Yeh, 1981).

If you create multiple input data files through node 7 (Figure 1) for making multiple runs, Block 3 will be repeated for each run as shown by the looping connection between node 11 and node 8 (Figure 1). An example of using Block 3 is given in Appendix 1.

(4) Block 4

This block is similar to Block 3 with the exception that a prompt (node 16) will appear at the end of each run to allow you the option of entering another run-ready input file name, if you want to make multiple runs. An example of using Block 4 is given in Appendix 2.

IV. SAMPLE ILLUSTRATIONS

To demonstrate what you may obtain from the use of AT123DIN and AT123DOUT, the following selected examples are presented:

TABLE 2: Shows the content of the AT123D input default data file, generated by AT123DIN, (Appendix 1).

TABLE 3: A listing of the content of VAR ID, VAR NAME, and VAR UNIT contained in the Type (i) dataset, TESTDATASET1, which was generated by AT123DOUT, (Appendix 1).

TABLE 4: Similar to Table 3, but retrieved from the Type (ii) dataset, TESTDATASET2.

TABLE 5: Similar to Table 3 or 4, but retrieved from the Type (iii) dataset, TESTDATASET3.

FIGURE 2: An x-y plane isopleth map created by extracting information contained in the Type (iii) dataset, TESTDATASET3. For this x-y plane plot, the time and z-coordinate specified were TIME=25000.0 hr and Z=10.0 meters.

FIGURE 3: This is an x-z plane isopleth map created by extracting information contained in the Type (iii) dataset, TESTDATASET3. For this x-y plane plot, the time and y-coordinate specified were TIME=25000.0 hr and Y=0.0 meters.

It is beyond the scope of this document to describe the application of GEMS' tabular, extraction, mapping, and other data management functions. Consult the User's Guide to GEMS (GSC, 1982) for detailed information.

V. SUMMARY

A concise guide to AT123D execution using GSC-developed input (AT123DIN) and output (AT123DOUT) data management systems is presented in this document. The basic AT123D input data groups are presented to provide the necessary background for the efficient use of AT123DIN and AT123DOUT. The execution logic is outlined by four major blocks, each of which you may invoke or bypass, using interactive commands. Most importantly, detailed examples (Appendix 1 and Appendix 2) with step-by-step explanatory comments are provided to guide you through a successful test AT123D execution. Follow those examples closely to ensure the most efficient use of the systems. Finally, sample illustrations are presented for demonstration purposes.

VI. ACKNOWLEDGEMENTS

The development of the AT123D execution supporting systems, AT123DIN and AT123DOUT, was sponsored by the Office of Pesticides and Toxic Substances of the U.S. Environmental Protection Agency. Helpful comments were received from Dr. Russell Kinerson and Dr. Annett Nold.

The following General Software Corporation staff participated in the AT123DIN and AT123DOUT systems development:

Project Manager: Jon Chen

Program Support: James Pilotte

System Support: Judy Chen

AT123DIN Programming: Dalroy Ward

AT123DOUT Programming: Yann King

AT123DIN Modifications: Stuart Wollman

REFERENCES

General Software Corp. 1982. User's guide to the Graphical Exposure Modeling System (GEMS). Draft report. Washington, DC: Office of Pesticides and Toxic Substances, U.S. Environmental Protection Agency. Contract 68016618.

Yeh, G.T. 1981, "AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System", ORNL-5602. Oak Ridge National Laboratory, Oak Ridge, TN.

TABLE 1. AT123DIN COMMANDS

The following is a list of commands that apply within AT123D. Note that all commands do not work at all prompts.

ALL	BACK	BRIEF	CANCEL	CLEAR	<CR>	DONE
EXIT	HELP	MENU	NOBRIEF	REVIEW		

for additional help with a command type: HELP <COMMAND>
for a full list of commands with explanations type: HELP *

ALL - for parameter input ALL designates that all parameters will be changed.

BACK - returns you to the previous prompt. NOTE: this command will not cancel any input that you have entered it simply allows you to return to a menu already looked at to make additional modifications.

BRIEF - no parameter descriptions will be given when a parameter menu is displayed.

CANCEL - cancels all input that you have entered and returns you to the first prompt(same as CLEAR).

CLEAR - cancels all input that you have entered and returns you to the first prompt.

<CR> - a carriage return assumes the currently selected data.

DONE - previous input and existing values are accepted and program execution continues with the next prompt.

EXIT - to end the AT123DIN program run.

HELP - provides command summary and descriptions.

MENU - displays the current parameter list when at a data item prompt.

NOBRIEF - allows display of parameter descriptions to be restored after BRIEF has been used.

REVIEW - allows you to review the current data.

TABLE 2. CONTENTS OF AT123D DEFAULT INPUT DATA FILE

```
TEST
   6    5    5  400    2    6    1    1    0    1    2    0    0    0    0    0
     0.00       0.00       0.00       1.00      -0.50       0.5       0.00       0.00
.30000001       0.1        0.01       1.00       0.1        0.1       0.00       0.00
     0.00       0.00    1320.00    1000.00       0.005   8760.00   43800.00       0.00
     0.00      10.00      20.00      30.00      40.00      50.00
   -10.00      -5.00       0.00       5.00      10.00
     0.00       5.00      10.00      15.00      20.00
```

NOTE: TITLE 'TEST' IS NOT A DEFAULT VALUE

TABLE 3. CONTENTS OF VAR ID, VAR NAME, AND VAR UNIT CONTAINED IN TESTDATASET1

Dataset name: TESTDATASET1 Length: 5

	VAR ID	VAR NAME	VAR UNIT
1	TIME	TIME OF SOLUTION	HRS
2	POLLUT	RESULTING POLLUTANT	PPM,PCI/ML,OR C
3	XPOINT	GIVEN X	METERS
4	YPOINT	GIVEN Y	METERS
5	ZPOINT	GIVEN Z	METERS

TABLE 4. CONTENTS OF VAR ID, VAR NAME, AND VAR UNIT CONTAINED IN TESTDATASET2

Dataset name: TESTDATASET2 Length: 5

	VAR ID	VAR NAME	VAR UNIT
1	Y/DIST	LOCATION IN X-DIREC.	METERS
2	POLLUT	RESULTING POLLUTANT	PPM,PCI/ML,OR C
3	TPOINT	GIVEN TIME	HRS
4	YPOINT	GIVEN Y	METERS
5	ZPOINT	GIVEN Z	METERS

TABLE 5. CONTENTS OF VAR ID, VAR NAME, AND VAR UNIT CONTAINED IN TESTDATASET3

Dataset name: TESTDATASET3 Length: 46

#	VAR ID	VAR NAME	VAR UNIT
1	TIME	TIME OF SOLUTION	HRS
2	XDIM	LOCATION IN X-DIREC.	METERS
3	YDIM	LOCATION IN Y-DIREC.	METERS
4	ZDIM	LOCATION IN Z-DIREC.	METERS
5	POLLUT	RESULTING POLLUTANT	PPM,PCI/ML,OR C
6	TITLE	JOB TITLE	-
7	NX	NO. OF POINTS IN X	-
8	NY	NO. OF POINTS IN Y	-
9	NZ	NO. OF POINTS IN Z	-
10	NROOT	NO. OF ROOTS	-
11	NBGTI	NO. OF BEGINNING DT	-
12	NEDTI	NO. OF ENDING DT	-
13	NPRINT	NO. OF DT FOR OUTPUT	-
14	INSTAN	SOURCE TYPE INDEX	-
15	NSOURS	SOURCE LOADING INDEX	-
16	INTER	INTERM. OUTPUT INDEX	-
17	ICASE	RUN TYPE INDEX	-
18	DEPTH	AQUIFER DEPTH	METERS
19	WIDTH	AQUIFER WIDTH	METERS
20	RL1	BEGIN OF SOURCE IN X	METERS
21	RL2	END OF SOURCE IN X	METERS
22	RB1	BEGIN OF SOURCE IN Y	METERS
23	RB2	END OF SOURCE IN Y	METERS
24	RH1	BEGIN OF SOURCE IN Z	METERS
25	RH2	END OF SOURCE IN Z	METERS
26	POR	POROSITY	-
27	HCOND	HYDRA. CONDUCT.	METER/HOUR
28	HGRAD	HYDRA. GRADIENT	-
29	AELONG	DESPERSIVITY IN Y	METERS
30	ATRANV	DESPERSIVITY IN Y	METERS
31	AVERTI	DESPERSIVITY IN Z	METERS
32	AKD	DISTRIBUTION COEF.	M**3/KG
33	AKE	HEAT EXCHANGE COEF.	KCAL/HR-M**2-C
34	AMTAU	MOLE DIFFUSION COEF.	M**2/HR
35	RAMADA	DECAY CONSTANT	PER HR
36	RHOP	SOIL BULK DENSITY	KG/M**3
37	RHOW	WATER DENSITY	KG/M**3
38	ACCU	ACCURANCY TOLERANCE	-
39	DT	TIME INTERVAL	HR
40	TDISP	DISCHARGE DURATION	HR
41	Q	WASTE RELEASE RATE	KG/,KCAL/,CI/HR
42	RETARD	RETARDATION FACTOR	-
43	UF	RETARDED DARCY VELO.	M/HR
44	AKX	RETARD DISP. COEF(X)	M**2/HR
45	AKY	RETARD DISP. COEF(Y)	M**2/HR
46	AKZ	RETARD DISP. COEF(Z)	M**2/HR

FIGURE 1. FLOWCHART FOR AT123D EXECUTION WITH DATA MANAGEMENT SYSTEM SUPPORT

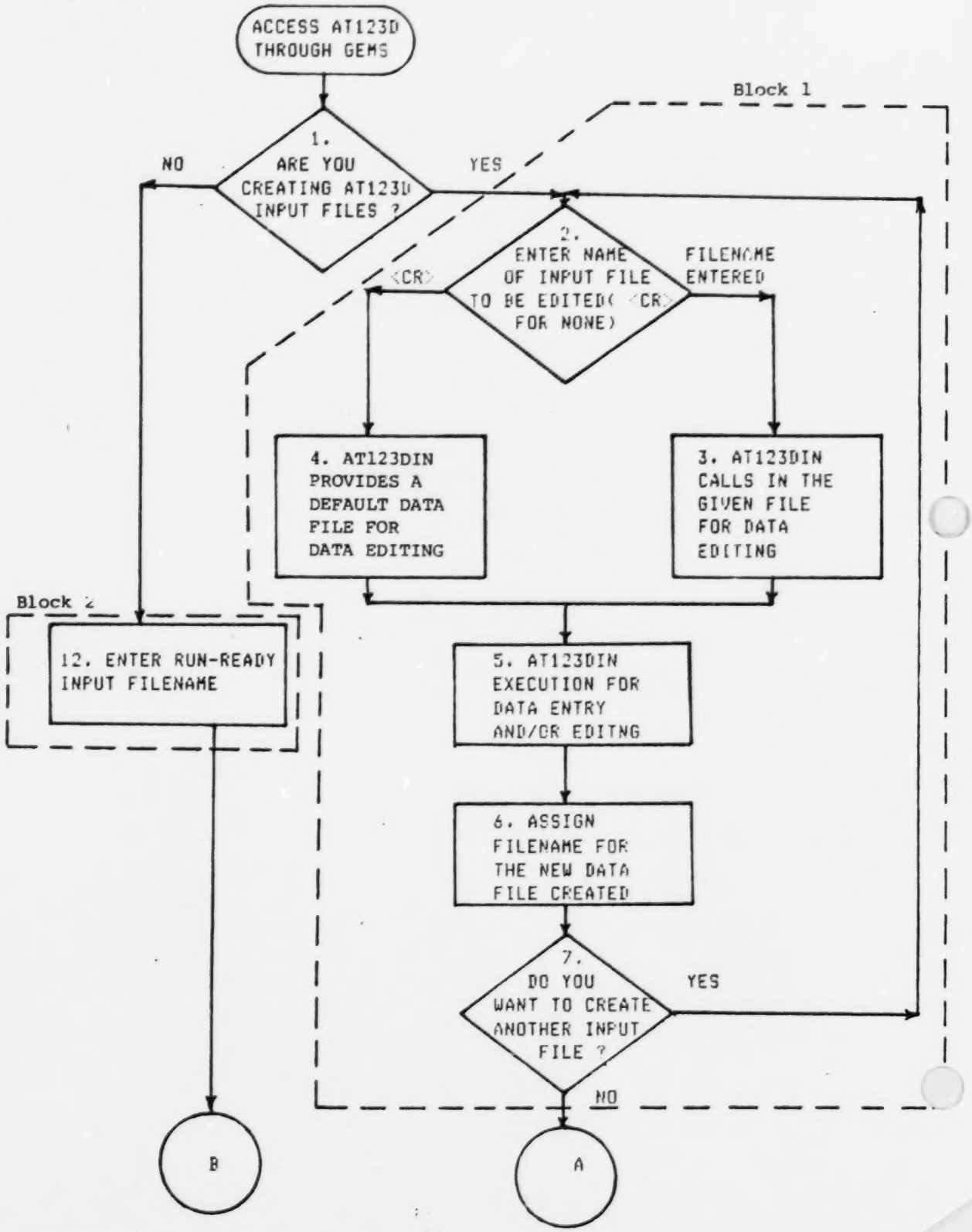

ACCESS AT123D THROUGH GEMS
Block 1
1. ARE YOU CREATING AT123D INPUT FILES ?
NO
YES
2. ENTER NAME OF INPUT FILE TO BE EDITED(<CR> FOR NONE)
<CR>
FILENAME ENTERED
4. AT123DIN PROVIDES A DEFAULT DATA FILE FOR DATA EDITING
3. AT123DIN CALLS IN THE GIVEN FILE FOR DATA EDITING
Block 2
12. ENTER RUN-READY INPUT FILENAME
5. AT123DIN EXECUTION FOR DATA ENTRY AND/OR EDITNG
6. ASSIGN FILENAME FOR THE NEW DATA FILE CREATED
7. DO YOU WANT TO CREATE ANOTHER INPUT FILE ?
YES
NO
B
A

FIGURE 1. FLOWCHART FOR AT123D EXECUTION WITH DATA MANAGEMENT SYSTEM SUPPORT(CONT'D)

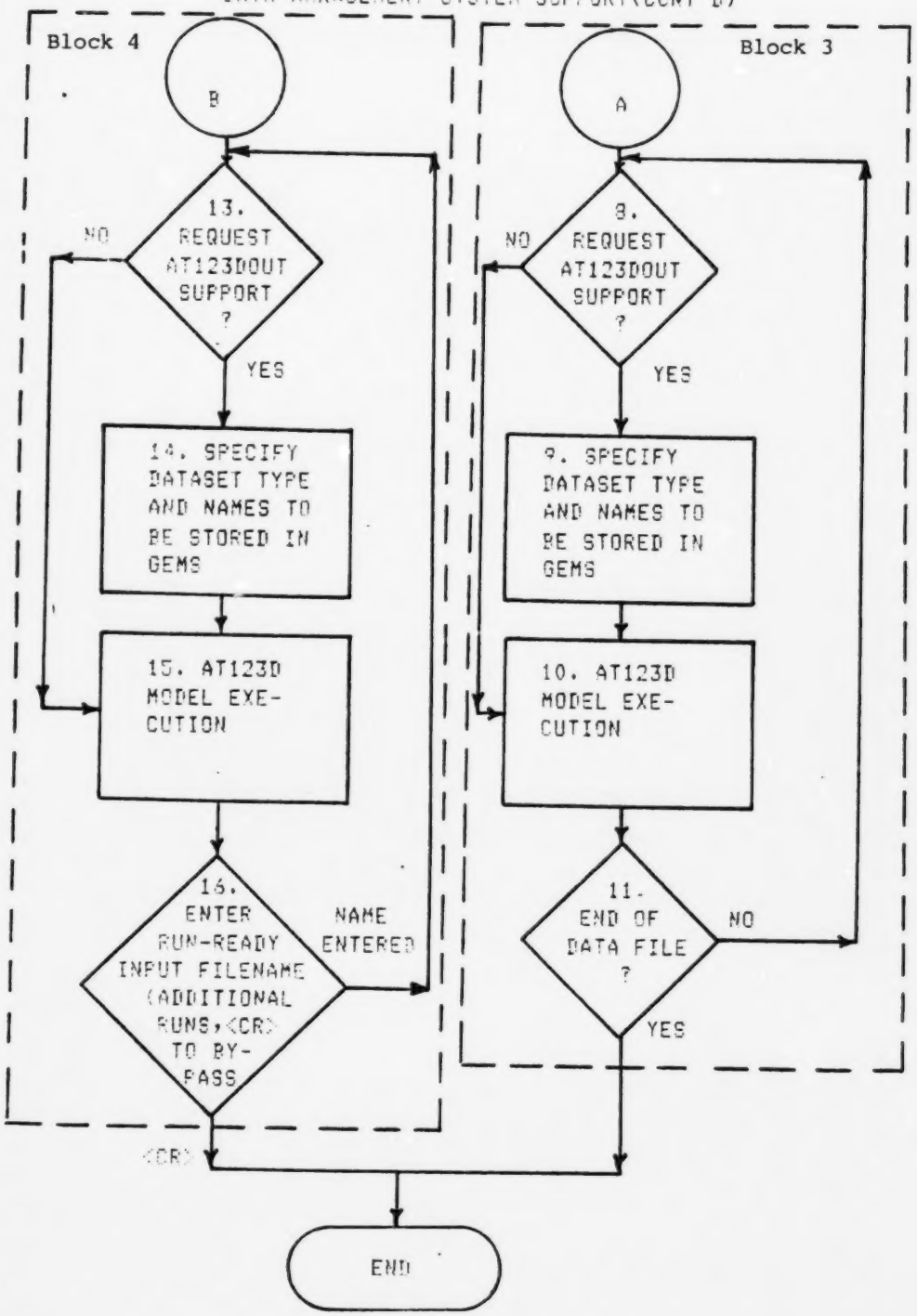


FIGURE 2. X-Y ISOPLETH MAP(TIME=25000,Z=10)

CONCENTRATION

From dataset TESTDATASET3

ISOPLETH #	VALUE (ppm)
1	2.20E+01
2	2.00E+01
3	1.80E+01
4	1.40E+01
5	1.00E+01
6	8.00E+00
7	6.00E+00
8	4.00E+00
9	2.50E+00
10	1.00E+00
11	5.00E-01

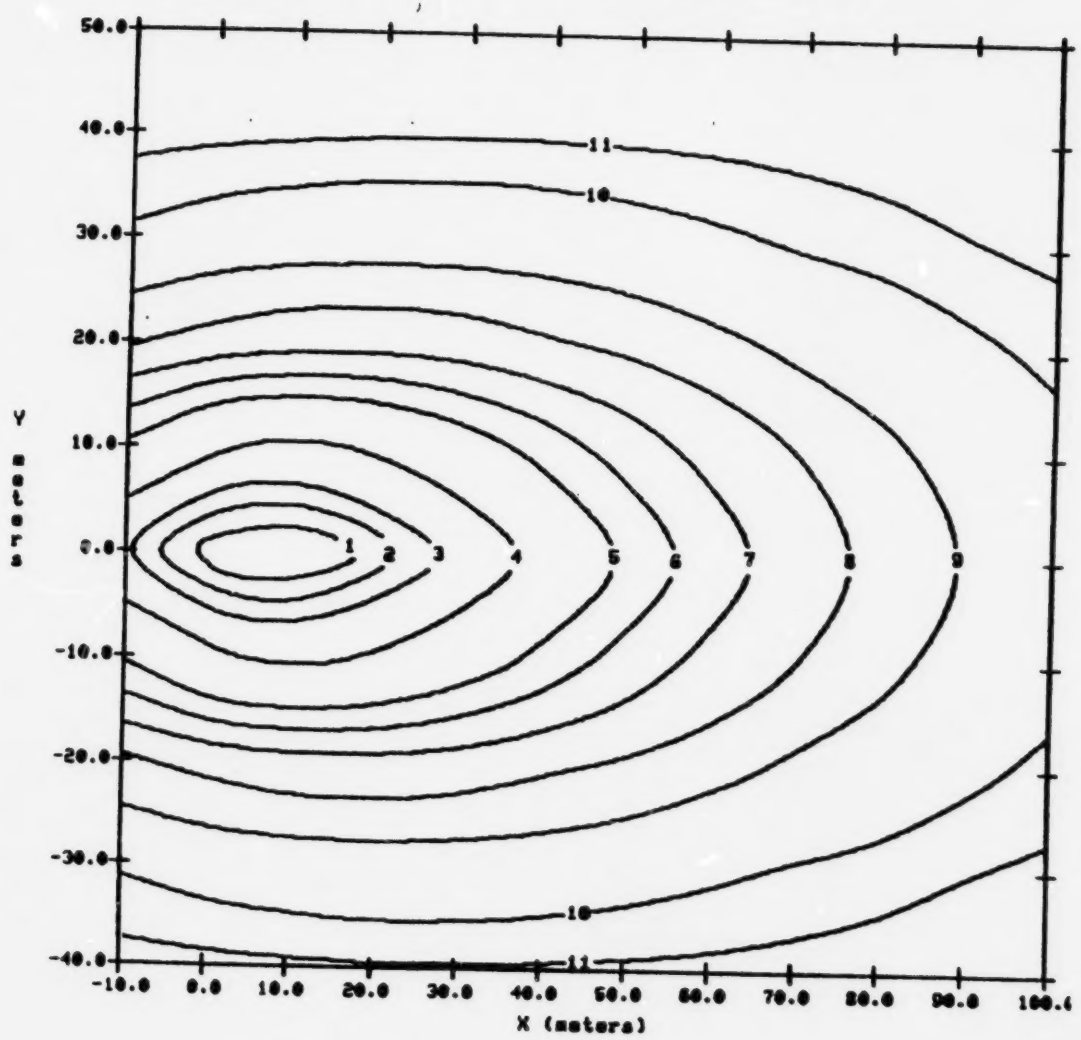
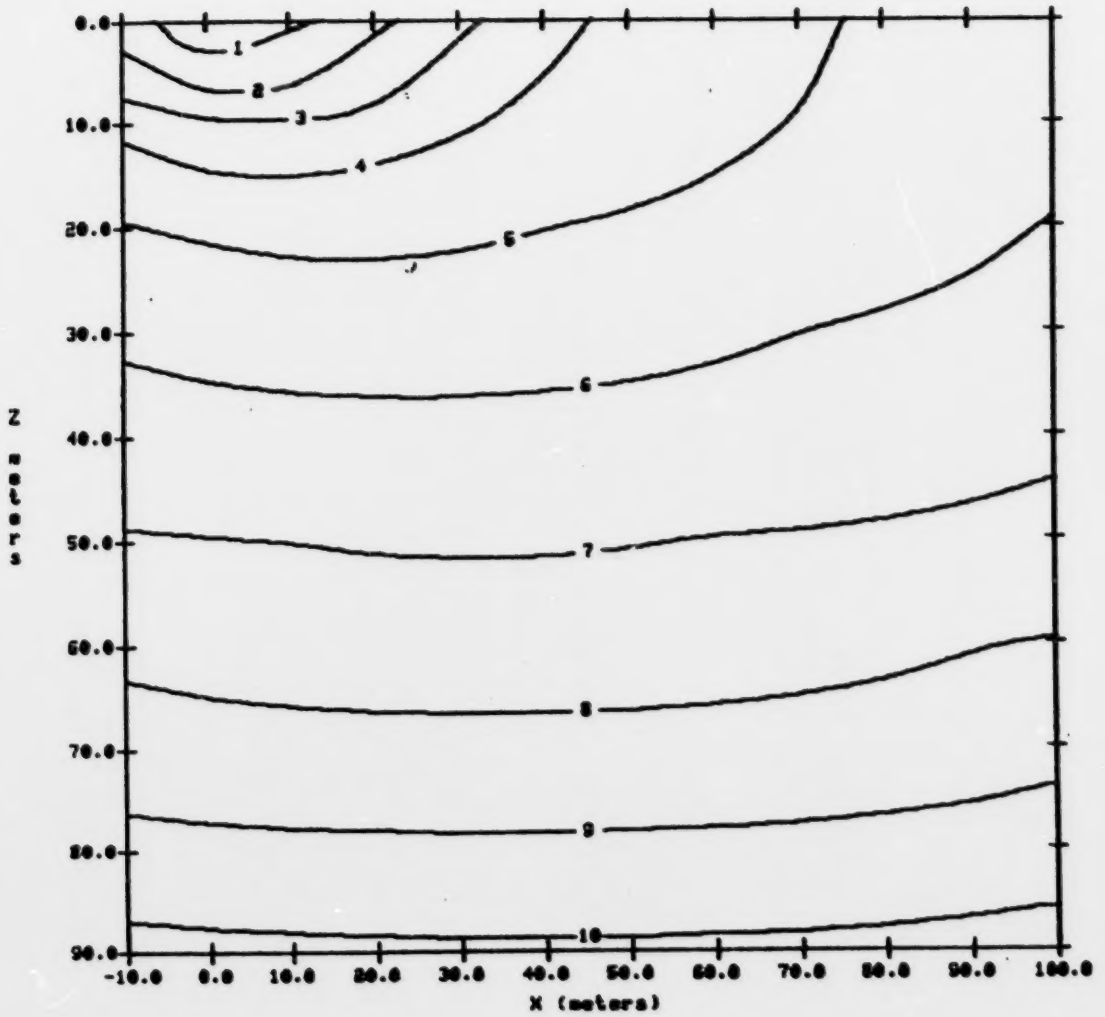


FIGURE 3. X-Z ISOPLETH MAP(TIME=25000,Y=0)

CONCENTRATION

From dataset TESTDATASET3

ISOPLETH #	VALUE (ppm)
1	6.00E+01
2	4.00E+01
3	2.50E+01
4	1.50E+01
5	5.00E+00
6	1.00E+00
7	1.00E-01
8	1.00E-02
9	1.00E-03
10	1.00E-04



APPENDIX 1: AT123D SAMPLE RUN USING AT123DIN AND AT123DOUT

Enter an operation: [m]

Enter a model name: [at123d]

NOTE
****
These are the two steps required
to access AT123D through GEMS.
[ ] encloses your response.

Are you creating (or modifying) AT123D input files(Y/N): [y]

NOTE
****
This is the decision to enter
either Block 1 or Block 2 of
Figure 1. Here, Block 1 is
entered. (Note that the term
'modifying' is included in the
prompt, since creating an input
file is done by modifying an
existing file.)

AT123DIN
INTERACTIVE AT123D INPUT
GSC VER1.1
10-DEC-84

For a list of commands type: HELP COMMANDS

Enter name of input file (<CR> for none) [<CR>]

NOTE
****
<CR> indicates that the default
data file is requested. The
new input data file will be
created by editing this default
data file. Otherwise, an existing
data file can be called in by
specifying the filename.

Enter TITLE for this run: [test]
New title: TEST

NOTE
****
A title is given to the data file.

NOTE: X - horizontal downgradient coordinate
Y - horizontal transverse coordinate
Z - depth below water table
DT - time step between computed solutions

BASIC INTEGER CONTROL PARAMETERS

1.	NX	Number points in x direc where solution wanted
2.	NY	Number points in y direc where solution wanted
3.	NZ	Number points in z direc where solution wanted
4.	NROOT	Number eigenvalues required for series evaluation
5.	NBGTI	Beginning time step number in terms of DT (must be >0)
6.	NEDTI	Ending time step number in terms of DT (must be >1)
7.	NPRINT	Every NPRINT time steps the solution is printed
8.	INSTAN	0 = instantaneous release, 1 = continuous release
9.	NSOUS	0 = constant source, >0 = number data points required
10.	INTER	are intermittant solutions to be printed 0 = no, 1 = yes
11.	ICASE	type of waste: 1 = heat, 2 = chemical, 3 = radioactive
12.	IWID	is media infinite in y direction: 0 = yes, 1 = no
13.	IDEP	is aquifer infinitely deep: 0 = yes, 1 = no

Select an item: [brief]

NOTE
****
Prior to selecting an item for editing, 'brief' is used to suppress the menu parameter descriptions. This will save editing time for experienced users.

Select an item: [menu]

NOTE
****
'menu' is used to get a listing of the group of parameters which are currently being edited.

1. NX
2. NY
3. NZ

```
    4.  NROOT
    5.  NRGTI
    6.  NEQTI
    7.  NPRINT
    8.  INSTAN
    9.  NSOUS
   10.  INTER
   11.  ICASE
   12.  IWID
   13.  IDEP

                        NOTE
                ********************************
                As shown, 'brief' is in effect.
                ('nobrief' can be used to turn
                off 'brief'.)


Select an item: [review]

                        NOTE
                ********************************
                'review' is used to examine the
                input data file in its entirety.


TEST
   6    5    5  400    2    6    1    1    0    1    2    0    0    0    0    0
     0.00       0.00       0.00       1.00      -0.50       0.5       0.00       0.00
.30000001       0.1        0.01       1.00       0.1        0.1       0.00       0.00
     0.00       0.00    1320.00    1000.00       0.005   8760.00   43800.00       0.00
     0.00      10.00      20.00      30.00      40.00      50.00
   -10.00      -5.00       0.00       5.00      10.00
     0.00       5.00      10.00      15.00      20.00

                        NOTE
                ********************************
                Since only the title has been
                changed up to now, the input
                data file shown is the default
                data file.


Select an item: [9]

The current value for NSOUS  is      0

Enter the new value: [8]

                        NOTE
                ********************************
                Here, the value of NSOUS was
                changed from 0 to 9.
```

Select an item: [done]

NOTE
****
'done' indicates that you are finished editing the current parameter group, and the editing proceeds to the next group.

AQUIFER SIZE AND SOURCE SIZE

1. DEPTH
2. WIDTH
3. RL1
4. RL2
5. RB1
6. RB2
7. RH1
8. RH2

Select an item: [depth]

NOTE
****
A parameter value may be called for editing by entering its name as well as its number.

The current value for DEPTH is 0.00 meters

Enter the new value: [100.]

Select an item: [3]

The current value for RL1 is 0.00 meters

Enter the new value: [-10.0]

Select an item: [done]

SOIL AND WASTE PROPERTIES

1. POR
2. HCOND
3. HGRAD
4. AELONG

```
   5.  ATRANV
   6.  AVERTI
   7.  AKD
   8.  AKE

Select an item: [back]

                        NOTE
                ********************************
                'back' is used here to return
                to the previous data group for
                additional editing.


AQUIFER SIZE AND SOURCE SIZE

   1.  DEPTH
   2.  WIDTH
   3.  RL1
   4.  RL2
   5.  RB1
   6.  RB2
   7.  RH1
   8.  RH2

Select an item: [3]

The current value for RL1       is      -10.00 meters

Enter the new value: [0.0]

                        NOTE
                ********************************
                RL1 is changed back to its
                original value of 0.0.


Select an item: [done]


SOIL AND WASTE PROPERTIES

   1.  POR
   2.  HCOND
   3.  HGRAD
   4.  AELONG
   5.  ATRANV
   6.  AVERTI
   7.  AKD
   8.  AKE

Select an item: [help]
```

Select one of the variables listed to be modified. A variable can be selected either by typing its name or its index number. To modify all variables in the menu (in order) type ALL. To go on to the next menu type DONE. To look at the menu again type MENU.

NOTE
****
As shown, 'help' is used to find
the proper response to the prompt:
'Select an item'.

Select an item: [all]

NOTE
****
'all' is used to indicate that
all of the parameters of this
group are to be changed.

The current value for POR is 0.30000001 [-]

Enter the new value: [.35]

The current value for HCOND is 0.1 M/HR

Enter the new value: [.15]

The current value for HGRAD is 0.01 [-]

Enter the new value: [.05]

The current value for AELONG is 1.00 M

Enter the new value: [2.00]

The current value for ATRANV is 0.1 M

Enter the new value: [.5]

The current value for AVERTI is 0.1 M

Enter the new value: [.5]

The current value for AKD is 0.00 M**3/KG

Enter the new value: [.0031]

The current value for AKE is 0.00 KC/HRM2C

Enter the new value: [<CR>]

NOTE
****
<CR> indicates that the current value of the parameter is not changed.

Select an item: [done]

ADDITIONAL SOIL AND WASTE PROPERTIES

1. AMTAU
2. RAMADA
3. RHOS
4. RHOW
5. ACCU
6. DT
7. TDISP
8. Q

Select an item: [done]

NOTE
****
No change has been made to this group.

X,Y,Z COORDINATES

1. XDIM
2. YDIM
3. ZDIM

Select an item: [nobrief]

NOTE
****
'nobrief' turns off the brief command, and parameter descriptions will be displayed with the menu listings.

Select an item: [done]

VARYING WASTE RELEASE RATE

1. QS kg/hr waste release rate at time = (I-1)*DT

Select an item: [1]

```
QS(  1)=      0.00 QS(  2)=      0.00 QS(  3)=      0.00 QS(  4)=      0.00
QS(  5)=      0.00 QS(  6)=      0.00 QS(  7)=      0.00 QS(  8)=      0.00

                              NOTE
                    ********************************
                    The number of elements displayed
                    in the array QS is equal to the
                    value of NSOUS in the second
                    parameter group. (all of the
                    elements are initially given the
                    the default value of 0.0)

Enter index to alter: [all]

                              NOTE
                    ********************************
                    The parameter values of all of
                    the elements of the array QS are
                    to be changed.

The current value for QS  ( 1) is       0.00 kg/hr

Enter the new value: [5.0]

The current value for QS  ( 2) is       0.00 kg/hr

Enter the new value: [5.0]

The current value for QS  ( 3) is       0.00 kg/hr

Enter the new value: [5.0]

The current value for QS  ( 4) is       0.00 kg/hr

Enter the new value: [7.0]

The current value for QS  ( 5) is       0.00 kg/hr

Enter the new value: [7.0]

The current value for QS  ( 6) is       0.00 kg/hr

Enter the new value: [7.0]

The current value for QS  ( 7) is       0.00 kg/hr

Enter the new value: [5.0]

The current value for QS  ( 8) is       0.00 kg/hr

Enter the new value: [5.0]
```

```
QS(  1)=      5.00 QS(  2)=      5.00 QS(  3)=      5.00 QS(  4)=      7.00
QS(  5)=      7.00 QS(  6)=      7.00 QS(  7)=      5.00 QS(  8)=      5.00
```

NOTE
****
The array QS is displayed with its new values.

```
Enter index to alter: [done]

Enter filename for new input file: [test.dat]
```

NOTE
****
This is to give a name to the input file just created.

```
Do you want to create another file? [no]
```

NOTE
****
A yes will set the program to create another input data file for multiple runs. The number of multiple runs is unlimited.

```
Do you want to run AT123D?: [yes]
```

NOTE
****
You have the option of running AT123D now or saving the newly created input data file(s) to run at a later time. A 'no' response here would do the latter.

```
Enter BATCH or INTERACTIVE : [i]
```

NOTE
****
An option to submit the run as interactive or batch type. Here, interactive mode is chosen.

```
ENTER Y TO REQUEST AT123DOUT SUPPORT > [y]
```

```
                        NOTE
                ********************************
                This is to decide if AT123DOUT
                support is needed(Block 3 of
                Figure 1).  Use of <CR> or
                symbols other than 'Y' will
                pass up the request.


ENTER Y IF YOU NEED POLLUTANT VS TIME PLOT AT A
SPECIFIED LOCATION > [y]

                        NOTE
                ********************************
                This is to decide if a type(i)
                dataset(Pollutant-Time plot) is
                needed.  Once the request is made
                (i.e. 'y' entry), you must
                respond to the 5 prompts below.


ENTER THE VALUES BELOW(FOR X,Y,&Z, THEY MUST BE
IN THE RANGE OF XDIM,YDIM,OR ZDIM,RESPECTIVELY):


HORIZ. DOWNGRADIENT DISTANCE(X)(METERS) >   [30.0]

                        NOTE
                ********************************
                If the value is not one of those
                in XDIM, the program will select
                one in XDIM nearest to the value
                entered.  Similar rules apply to
                the Y,Z, and TIME entries below.


HORIZ. TRANSVERSE DIST.(Y)(METERS)(ENTER 999.9
TO GET DEFAULT VALUE AT THE CENTER OF PLUME) >  [999.9]

                        NOTE
                ********************************
                '999.9' can be used to set the
                POLLUTANT-TIME plot along the
                centerline of the plume.


DEPTH BELOW WATER TABLE(Z)(METERS) >   [10.0]


GEMS DATASET NAME(1 TO 12 CHARACTERS) > [testdataset1]
```

NOTE
****
A name is given to this dataset
which is to be stored in GEMS.

TAG FIELD(1 TO 60 CHARAC., HIT <CR> TO BYPASS > [sample pollutant time plot]

NOTE
****
The tag field gives more descriptive information about the dataset stored in GEMS. Bypass can be made by entering <CR>.

ENTER Y IF YOU NEED ANOTHER POLLUTANT VS TIME PLOT
AT A SPECIFIED LOCATION > [<CR>]

NOTE
****
Another Type(i) dataset can be created. <CR> bypasses this option.

ENTER Y IF YOU NEED POLLUTANT VS X-DIST. PLOT AT A
SPECIFIED TIME,Y,Z LOCATIONS > [y]

NOTE
****
This is to decide if a Type(ii) dataset(POLLUTANT-XDIST plot) is needed.

ENTER THE VALUES BELOW(FOR X,Y,Z, THEY MUST BE
IN THE RANGE OF XDIM,YDIM,OR ZDIM,RESPECTIVELY):

DESIRED TIME(HRS)(NEAREST TIME WILL BE SELECTED
BASED ON YOUR NPRINT AND DT VALUES) > [17520.]

NOTE
****
Here, the POLLUTANT-XDIST plot is requested at time=17520 hr. (2 years).

HORIZ. TRANSVERSE DIST.(Y)(METERS)(ENTER 999.9
TO GET DEFAULT VALUE AT THE CENTER OF PLUME) > [999.9]

APP.1: AT123D SAMPLE RUN USING AT123DIN AND AT123DOUT(CONT'D)

```
GEMS DATASET NAME(1 TO 12 CHARACTERS) > [TESTDATASET2]

                        NOTE
                ******************************
                This is the name assigned to
                the POLLUTANT-XDIST plot dataset
                requested above.

TAG FIELD(1 TO 60 CHARAC., HIT <CR> TO BYPASS > [sample pollutant x-dist plot]

ENTER Y IF YOU NEED ANOTHER POLLUTANT VS X-DIST. PLOT
AT A SPECIFIED TIME & Y,Z LOCATIONS > [<CR>]

                        NOTE
                ******************************
                Another Type(ii) dataset could
                be requested here.  The total
                number of Type(i),(ii), and (iii)
                datasets requested in one run
                cannot exceed 10.


ENTER Y IF YOU NEED STORING ALL AT123D OUTPUT IN GEMS
(NOTE-- TO AVOID WASTE OF LARGE STORAGE SPACE, REQUEST OF
THIS SUPPORT IS DISCOURAGED UNLESS YOU HAVE DEFINITE NEED
OF THIS LARGE DATASET) > [y]

                        NOTE
                ******************************
                The type(iii) dataset(all data
                stored in GEMS) is requested
                here.


GEMS DATASET NAME(1 TO 12 CHARACTERS) > [testdataset3]

TAG FIELD(1 TO 60 CHARAC., HIT <CR> TO BYPASS > [all test output data storage]

                        NOTE
                ******************************
                The program is running at this
                stage, and a presentation of
                all the GEMS datasets requested
                is displayed below.


  DSNAME(P VS TIME) =TESTDATASET1
  DSNAME(P VS X   ) =TESTDATASET2
  DSNAME(ALL DATA ) =TESTDATASET3
```

```
Enter a model name:

                        NOTE
                ******************************
                This is back to GEMS.



**************************NOTE*****************************
*************************************************************
In summary, this example shows the use of both AT123DIN
and AT123DOUT in making an AT123D run.  The default
input data file was edited to create the following new
input data file for execution: TEST.DAT

Through AT123DOUT, the three datasets: TESTDATASET1,
TESTDATASET2, and TESTDATASET3 were created and stored
GEMS for later analysis.  The complete AT123D output is
presented in a file named AT123DOUT.DAT

For multiple runs, the outputs will be presented in terms
of different versions of the AT123DOUT.DAT files.
For example:
              AT123DOUT.DAT;1 for run no. 1
              AT123DOUT.DAT;2 for run no. 2
              AT123DOUT.DAT;3 for run no. 3
                      .               .
                      .               .
                      .
This example has demonstrated  the use of most of the
available AT123DIN commands.  However, the following ones
are left for your exercise: CLEAR, HELP COMMANDS, HELP *,
EXIT.
*************************************************************
```

APPENDIX 2: AT123D SAMPLE RUN BYPASSING AT123DIN AND AT123DOUT

```
Enter an operation: [m]

Enter a model name: [at123d]
```

NOTE
****
These are the two steps required to access AT123D through GEMS. [ ] encloses your response.

```
Are you creating (or modifying) AT123D input files(Y/N): [n]
```

NOTE
****
This is the decision to enter either Block 1 or Block 2 of Figure 1. As shown, Block 2 is entered here.

```
Enter run-ready input filename : [test.dat]
```

NOTE
****
Since AT123DIN support is not requested here, the run-ready filename must be entered for execution. Here, the input data file TEST.DAT created in Appendix 1 is used.

```
ENTER Y TO REQUEST AT123DOUT SUPPORT > [<CR>]
```

NOTE
****
AT123DOUT support is not requested here. The program is executing at this stage.

```
Enter run-ready input filename(another run,<cr> to bypass): [<CR>]
```

NOTE
****
The first run has been completed. The option for making another run is given here. Input a file name for another run or <CR> to bypass.

APP.2: AT123D SAMPLE RUN BYPASSING AT123DIN AND AT123DOUT

```
Enter a model name:

                              NOTE
                    ********************************
                    This is back to GEMS.


************************NOTE************************
****************************************************
In summary, this example shows the making of an
AT123D run without using AT123DIN and AT123DOUT.
The existing data file TEST.DAT was entered for
immediate execution.  The output of AT123D is
presented in a file named AT123DOUT.DAT.  For
multiple runs, the output will be presented in
terms of different versions of the AT123DOUT.DAT
files.  For example:
                AT123DOUT.DAT;1  for run no. 1
                AT123DOUT.DAT;2  for run no. 2
                AT123DOUT.DAT;3  for run no. 3
                        .              .
                        .              .
                        .              .
****************************************************
****************************************************
```

APPENDIX 3. PRESENTATION OF THE NINE INPUT DATA GROUPS OF AT123D AND THEIR DEFAULT VALUES

VAR.	NAME	VARIABLE DESCRIPTION AND UNITS	DEF. VALUE
o	Group 1:	Title	
	TITLE	Title of the job (up to 80 characters)	
o	Group 2:	Basic Integer Parameters	
	NX	Number of points in the x-direction (horizontal downgradient) where the solution is desired	6
	NY	Number of points in the y-direction (horizontal transverse) where the solution is desired	5
	NZ	Number of points in the z-direction (vertical downward) where the solution is desired	5
	NROOT	Number of eigenvalues required for series evaluation	400
	NBGTI	Number of beginning time step in terms of DT when the solution is desired	2
	NEDTI	Number of ending time step in terms of DT when the solution is desired	6
	NPRINT	An integer parameter indicating that for every NPRINT time steps the solution is desired	1
	INSTAN	An integer parameter indicating if the release is an instantaneous release or not: =0 instantaneous release, =1 continuous release	1
	NSOUS	An integer parameter indicating if the source release is constant or changing with time: =0 constant source ≠0 NSOUS data points as function of time is required (i.e. Group 9 data)	0
	INTER	An integer parameter indicating if intermittant solutions between NBGTI and NEDTI are to be line-printed: =0 no, =1 yes	1
	ICASE	An integer parameter indicating what type of waste is being simulated: =1 for heat, =2 for chemical, =3 for radwaste	2

VAR. NAME	VARIABLE DESCRIPTION AND UNITS	DEF. VALUE
IWID	An integer parameter indicating if the media is infinite or not in the y-direction: =0 yes, =1 no	0
IDEP	An integer parameter indicating if the aquifer is infinitely deep: =0 yes, =1 no	0
IBUG	An integer parameter indicating if the diagnostic check is desired or not: =0 no, =1, yes. For debugging, IBUG is normally set to 1. For production, IBUG is normally set to zero	0
o Group 3:	Aquifer Size and Source Size	
DEPTH	Aquifer depth (0 for infinite) (meters)	0
WIDTH	Aquifer width (0 for infinite) (meters)	0
RL1	Beginning coordinate of the source in the x-direction (meters)	0.0
RL2	Ending coordinate of the source in the x-direction (meters)	1.0
RB1	Beginning coordinate of the source in the y-direction (meters)	-0.5
RB2	Ending coordinate of the source in the y-direction (meters)	0.5
RH1	Beginning coordinate of the source in the z-direction (meters)	0.0
RH2	Ending coordinate of the source in the z-direction (meters)	0.0
o Group 4:	Soil and Waste Properties	
POR	Effective porosity of the soil	0.30
HCOND	Hydraulic conductivity (M/HR)	0.1
HGRAD	Hydraulic gradient	0.01

VAR. NAME	VARIABLE DESCRIPTION AND UNITS	DEF. VALUE
AELONG	Longitudinal dispersivity (meters)	1.0
ATRANV	Transverse dispersivity (meters)	0.1
AVERTI	Vertical dispersivity (meters)	0.1
AKD	Distribution coefficient (M**3/KG)	0.0
AKE	Modified heat exchange coefficient (KCAL/HR-M**2-^{o}C)	0.0
o Group 5:	More Soil and Waste Properties	
AMTAU	Molecular diffusion coefficient (M**2/HR)	0.0
RAMADA	Decay constant (1/HR)	0.0
RHOB	Bulk density of the soil (KG/M**3)	1320.0
RHOW	Density of water (KG/M**3)	1000.0
ACCU	Error tolerance if steady-state solution is desired	0.005
DT	Time step interval for which the solution is desired (HR)	8760.0
TDISP	Time duration of waste release (HR)	43800.0
Q	Constant waste release rate or total instantaneous release (KCAL/HR, KG/HR, or CI/HR)	0.0
o Group 6:	X-Space Coordinate	
XDIM(I)	The I-th coordinate in the x-direction where the solution is desired. (I=1, NX) (meters)	0.0
XDIM(1)		0.0
XDIM(2)		10.0
XDIM(3)		20.0
XDIM(4)		30.0

VAR. NAME	VARIABLE DESCRIPTION AND UNITS	DEF. VALUE
XDIM(5)		40.0
XDIM(6)		50.0
o Group 7:	Y-Space Coordinate	
YDIM(I)	The I-th coordinate in the y-direction where the solution is desired. (I=1, NY) (meters)	
YDIM(1)		-10.0
YDIM(2)		-5.0
YDIM(3)		0.0
YDIM(4)		5.0
YDIM(5)		10.0
o Group 8:	Z-Space Coordinate	
ZDIM(I)	The I-th coordinate in the z-direction where the solution is desired. (I=1, NZ) (meters)	
ZDIM(1)		0.0
ZDIM(2)		5.0
ZDIM(3)		10.0
ZDIM(4)		15.0
ZDIM(5)		20.0
o Group 9:	Variable Source Release Rate (required only if NSOUS≠0)	
QS(I)	The I-th waste release rate at time=(I-1)*DT, where I=1, NSOUS. (KCAL/HR, KG/HR, or CI/HR)	Not Used (NSOUS=0)